

# Evolution Equations in Functional Derivatives of Many-Particle Systems

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**Abstract.** The hierarchies of evolution equations of classical many-particle systems are formulated as evolution equations in functional derivatives. In particular the BBGKY hierarchy for marginal distribution functions, the dual BBGKY hierarchy for marginal observables, the Liouville hierarchy for correlation functions and the nonlinear BBGKY hierarchy for the marginal correlation functions are considered. The nonperturbative solution expansions of the Cauchy problem of these hierarchies are constructed on the basis of established relations between the generating functionals of corresponding functions. The obtained results are generalized on systems of particles interacting via many-body potentials.

**Key words:** BBGKY hierarchy; Liouville hierarchy; generating functional; functional derivative; marginal observable; marginal distribution function; correlation.

*2000 Mathematics Subject Classification:* 82C05; 82C22; 49S05; 47J30; 35Q82.

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## 1 Introduction

It is well known the meaning of methods of the functional differentiation and functional integration for the problems of mathematical physics [1, 2] and applications [3], in particular with regard to many-particle systems of statistical mechanics or quantum field theory. As far as we know for the first time equations in functional derivatives for the description of the evolution of states of many-particle systems were used by T.H. Gronwall [4], M.A. Leontovich [5] and N.N. Bogolyubov [6, 7]. Bogolyubov's results were developed by R.L. Lewis in the paper [8], where it was constructed the reduced representation of a nonperturbative solution of the Cauchy problem of the BBGKY hierarchy. On quantum many-particle systems Bogolyubov approach was extended in [9].

In this article we present the rigorous results on the evolution equations in functional derivatives for generating functionals of states and observables of classical many-particle systems, namely the BBGKY hierarchy and the dual BBGKY hierarchy in functional derivatives respectively [10]. One more approach to the description of the evolution of states of many-particle systems is given by means of generating functionals for correlation functions. The generating functionals of correlation functions and marginal correlation functions are governed by the von Neumann hierarchy and the nonlinear BBGKY hierarchy in functional derivatives respectively. On the basis of the developed approach we construct nonperturbative solutions of the Cauchy problem of corresponding evolution equations in appropriate Banach spaces.

We briefly outline the results and structure of the paper. In section 2 we set forth an approach to the description of the evolution of states of many-particle systems within the framework of the generating functional of marginal distribution functions governed by the BBGKY hierarchy in functional derivatives. Then by means of introduced generating functional of marginal distribution functions we construct a nonperturbative solution of the initial-value problem of the BBGKY hierarchy on the basis of cluster expansions of groups of operators which describe dynamics of finitely many particles.

In section 3 we develop an alternative method to the description of the evolution of states within the framework of the generating functionals of correlation functions and marginal correlation functions governed by the von Neumann hierarchy and the nonlinear BBGKY hierarchy in functional derivatives respectively. The relationships of the introduced generating functionals of states are established.

In section 4 we state an equivalent approach to the description of the evolution of many-particle systems within the framework of the generating functional of marginal observables governed by the dual BBGKY hierarchy in functional derivatives. A nonperturbative solution of the initial-value problem of the dual BBGKY hierarchy is constructed on the basis of cluster expansions of groups of operators which describe the evolution of observables.

Finally in section 5 we conclude with some observations and perspectives for future research.

## 2 The BBGKY hierarchy in functional derivatives

### 2.1 A generating functional of marginal distribution functions

Let  $f = (f_0, f_1(x_1), \dots, f_n(x_1, \dots, x_n), \dots)$  be a sequence of measurable functions defined on the phase spaces of the corresponding number of particles and  $u = (1, u(x_1), \dots, \prod_{i=1}^n u(x_i), \dots)$  is a sequence of products of continuously differentiable integrable functions  $u(x_i)$ ,  $i \geq 1$ . The generating functional of functions  $f_n$ ,  $i \geq 1$  is defined by the following expression

$$(f, u) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int f_n(x_1, \dots, x_n) \prod_{i=1}^n u(x_i) dx_1 \dots dx_n. \quad (1)$$

For the integrable functions  $u(x_i)$ ,  $i \geq 1$ , functional (1) exists. We refer to functional (1) as the generating functional of functions  $f_n(x_1, \dots, x_n)$ ,  $n \geq 1$ , by reason of the equality

$$f_n(x_1, \dots, x_n) = \frac{\delta^n}{\delta u(x_1) \dots \delta u(x_n)} (f, u) |_{u=0}, \quad (2)$$

where  $\delta^n / \delta u(x_1) \dots \delta u(x_n)$  is the  $n$ th order functional derivative (the  $n$ th order Gâteaux derivative [11, 12]).

We consider a system of a non-fixed number of particles in the space  $\mathbb{R}^3$  defined by the Hamiltonian [13]

$$H_n = \sum_{i=1}^n K(p_i) + \sum_{i < j=1}^n \Phi(q_i - q_j), \quad (3)$$

where  $K(p_i)$  is a kinetic energy of the  $i$  particle and  $\Phi(q_i - q_j)$  is a two-body interaction potential. Hereafter we assume that the function  $\Phi$  satisfies conditions which guarantee the existence of a global in time solution of the Hamilton equations for finitely many particles [13]. The evolution of states of a system is described by the sequence  $D(t) = (1, D_1(t, x_1), \dots, D_n(t, x_1, \dots, x_n), \dots)$  of distribution functions. The integrable function  $D_n(t, x_1, \dots, x_n)$  is defined on the  $n$ -particle phase space and symmetric with respect to the permutations of the arguments  $x_1, \dots, x_n$ . We introduce the generating functional  $(D(t), u)$  of the distribution functions  $D_n(t, x_1, \dots, x_n)$ ,  $n \geq 1$ , according to definition (1) by the expansion

$$(D(t), u) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int D_n(t, x_1, \dots, x_n) \prod_{i=1}^n u(x_i) dx_1 \dots dx_n. \quad (4)$$

The evolution of states of many-particle systems in terms of generating functional (4) is governed by the following evolution equation in functional derivatives

$$\begin{aligned} \frac{d}{dt}(D(t), u) = & \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)}(D(t), u) \right\} u(x_1) dx_1 + \\ & + \frac{1}{2!} \int \int \left\{ \Phi(q_1 - q_2), \frac{\delta^2}{\delta u(x_1) \delta u(x_2)}(D(t), u) \right\} u(x_1) u(x_2) dx_1 dx_2, \end{aligned} \quad (5)$$

where  $\{.,.\}$  is the Poisson bracket. Then taking into account equality (2), we observe that the distribution functions  $D_n(t)$ ,  $n \geq 1$ , are determined by a sequence of the Liouville equations

$$\frac{\partial}{\partial t} D_n(t) = \{H_n, D_n(t)\}, \quad n \geq 1. \quad (6)$$

We note that the inverse proposition is also true, namely the generating functional of solutions of the Liouville equations (6) satisfies equation (5). By reason of this we are referred to evolution equation (5) as the Liouville equation in functional derivatives.

We consider an equivalent approach to the description of the evolution of states of many-particle systems within the framework of a generating functional of marginal distribution functions [13]. To that end we introduce a generating functional of the marginal distribution functions  $F_s(t, x_1, \dots, x_s)$ ,  $s \geq 1$ , by means of generating functional (4)

$$(F(t), u) = (\tilde{D}(t), u + 1), \quad (7)$$

where  $\tilde{D}(t) = (D(t), I)^{-1}(1, D_1(t, x_1), \dots, D_n(t, x_1, \dots, x_n), \dots)$  is a sequence of normalized distribution functions,  $(D(t), I)$  is a normalizing factor (grand canonical partition function)

$$(D(t), I) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int D_n(t, x_1, \dots, x_n) dx_1 \dots dx_n,$$

and hence  $I \equiv (1, \dots, 1, \dots)$ . In consequence of introduced generating functional (7) we establish the relation between marginal distribution functions and distribution functions. For this purpose we transform the generating functional  $(\tilde{D}(t), u + 1)$  to form (1) to determine the sequence of functions generated by such functional. The following equality holds

$$(\tilde{D}(t), u + 1) = (e^a \tilde{D}(t), u), \quad (8)$$

where on  $f \in L^1$  the operator  $\mathfrak{a}$  (an analog of the annihilation operator [13]) is defined by the formula

$$(\mathfrak{a}f)_n(x_1, \dots, x_n) \doteq \int f_{n+1}(x_1, \dots, x_{n+1}) dx_{n+1}. \quad (9)$$

Indeed we have

$$\begin{aligned} (\tilde{D}(t), u+1) &= (D(t), I)^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int D_n(t, x_1, \dots, x_n) \prod_{i=1}^n (u(x_i) + 1) dx_1 \dots dx_n = \\ &= (D(t), I)^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int D_n(t, x_1, \dots, x_n) \sum_{k=0}^n \sum_{i_1 < \dots < i_k=1}^n u(x_{i_1}) \dots u(x_{i_k}) dx_1 \dots dx_n = \\ &= (D(t), I)^{-1} \sum_{s=0}^{\infty} \frac{1}{s!} \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int D_{s+n}(t, x_1, \dots, x_{s+n}) \prod_{i=1}^s u(x_i) dx_1 \dots dx_{s+n}. \end{aligned}$$

Therefore, according to (2), from (7) and (8) we obtain the expression for marginal distribution functions within the framework of nonequilibrium grand canonical ensemble [13]

$$F_s(t, x_1, \dots, x_s) = (D(t), I)^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int D_{s+n}(t, x_1, \dots, x_{s+n}) dx_{s+1} \dots dx_{s+n}.$$

Using the Liouville equation in functional derivatives (5), from relation (7) we derive the evolution equation in functional derivatives for the generating functional of marginal distribution functions

$$\begin{aligned} \frac{d}{dt}(F(t), u) &= \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)}(F(t), u) \right\} (u(x_1) + 1) dx_1 + \\ &+ \frac{1}{2!} \int \int \left\{ \Phi(q_1 - q_2), \frac{\delta^2}{\delta u(x_1) \delta u(x_2)}(F(t), u) \right\} \prod_{i=1}^2 (u(x_i) + 1) dx_1 dx_2. \end{aligned} \quad (10)$$

We are referred to this equation as the BBGKY hierarchy in functional derivatives [6–8]. Taking into account equality (2), from evolution equation (10) we establish that the marginal distribution functions  $F_s(t)$ ,  $s \geq 1$ , are determined by the BBGKY hierarchy

$$\frac{\partial}{\partial t} F_s(t) = \{H_s, F_s(t)\} + \int \left\{ \sum_{i=1}^s \Phi(q_i - q_{s+1}), F_{s+1}(t) \right\} dx_{s+1}, \quad s \geq 1. \quad (11)$$

As above in case of the the Liouville equations (6) the generating functional of solutions of the BBGKY hierarchy (11) satisfies equation (10).

To clarify the structure of stated above evolution equations in functional derivatives we generalize them for systems of particles interacting via many-body interaction potentials

$$H_n = \sum_{i=1}^n K(p_i) + \sum_{k=1}^n \sum_{1=i_1 < \dots < i_k}^n \Phi^{(k)}(q_{i_1}, \dots, q_{i_k}), \quad n \geq 1, \quad (12)$$

where  $\Phi^{(k)}$  is a  $k$ -body interaction potential. In this case the Liouville equation in functional derivatives has the form

$$\begin{aligned} \frac{d}{dt}(D(t), u) = & \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)}(D(t), u) \right\} u(x_1) dx_1 + \\ & + \sum_{n=1}^{\infty} \frac{1}{n!} \int \dots \int \left\{ \Phi^{(n)}(q_1, \dots, q_n), \frac{\delta^n}{\delta u(x_1) \dots \delta u(x_n)}(D(t), u) \right\} \prod_{i=1}^n u(x_i) dx_1 \dots dx_n, \end{aligned} \quad (13)$$

and distribution functions are determined by a sequence of the Liouville equations (6) with the Hamiltonian (12) respectively.

The BBGKY hierarchy in functional derivatives for the generating functional of marginal distribution functions takes the form

$$\begin{aligned} \frac{d}{dt}(F(t), u) = & \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)}(F(t), u) \right\} (u(x_1) + 1) dx_1 + \\ & + \sum_{n=1}^{\infty} \frac{1}{n!} \int \dots \int \left\{ \Phi^{(n)}(q_1, \dots, q_n), \frac{\delta^n}{\delta u(x_1) \dots \delta u(x_n)}(F(t), u) \right\} \prod_{i=1}^n (u(x_i) + 1) dx_1 \dots dx_n, \end{aligned} \quad (14)$$

and the marginal distribution functions are determined by the BBGKY hierarchy respectively

$$\begin{aligned} \frac{\partial}{\partial t} F_s(t) = & \{H_s, F_s(t)\} + \sum_{k=1}^s \frac{1}{k!} \sum_{i_1 \neq \dots \neq i_k=1}^s \sum_{n=1}^{\infty} \frac{1}{n!} \int \dots \int \left\{ \Phi^{(k+n)}(q_{i_1}, \dots, q_{i_k}, \right. \\ & \left. q_{s+1}, \dots, q_{s+n}), F_{s+n}(t) \right\} dx_{s+1} \dots dx_{s+n}, \quad s \geq 1. \end{aligned} \quad (15)$$

We can see that the structure of the Liouville equation and the BBGKY hierarchy in functional derivatives is similar in contrast to the structure of these equations for corresponding distribution functions.

## 2.2 A nonperturbative solution of the BBGKY hierarchy

On the basis of a solution of the Liouville equation (6) and relation (7) for generating functionals, we construct a nonperturbative solution of the Cauchy problem of the BBGKY hierarchy (11). We consider the sequence

$$\tilde{D}(t) = (S(-t)D(0), I)^{-1}(1, (S_1(-t)D_1(0))(x_1), \dots, (S_n(-t)D_n(0))(x_1, \dots, x_n), \dots),$$

where  $S_n(-t)$ ,  $t \in \mathbb{R}$ , is the group of evolution operators defined on the space  $L_n^1$  by the formula

$$(S_n(-t)f_n)(x_1, \dots, x_n) \doteq f_n(X_1(-t, x_1, \dots, x_n), \dots, X_n(-t, x_1, \dots, x_n)), \quad (16)$$

where  $X_i(-t, x_1, \dots, x_n)$ ,  $1 \leq i \leq n$ , are solutions of the Cauchy problem of the Hamilton equations of  $n$  particle system with initial data:  $x_1, \dots, x_n$ . The function  $S_n(-t)D_n(0)$  is a solution of the Cauchy problem of the Liouville equation (6) with the initial data  $D_n(0)$  [13].

In the functional  $(e^a S(-t)D(0), u)$  we expand operators (16) over their cumulants as the following cluster expansions

$$S_{s+n}(-t, Y, X \setminus Y) = \sum_{P: \{Y\}, X \setminus Y = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(-t, X_i), \quad n \geq 0, \quad (17)$$

where  $Y \equiv (x_1, \dots, x_s)$ ,  $(\{Y\})$  is the set consisting of one element  $Y = (x_1, \dots, x_s)$ ,  $X \equiv (x_1, \dots, x_{s+n})$ , and  $\sum_{P: (\{Y\}, X \setminus Y) = \bigcup_i X_i}$  is the sum over all possible partitions  $P$  of the set  $(\{Y\}, X \setminus Y)$  into  $|P|$  nonempty mutually disjoint subsets  $X_i \subset (\{Y\}, X \setminus Y)$ . Owing to the equality

$$\sum_{P: (\{Y\}, X \setminus Y) = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(-t, X_i) = \sum_{Z \subset X \setminus Y} \mathfrak{A}_{1+|Z|}(-t, \{Y\}, Z) \sum_{P: X \setminus Y \setminus Z = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(-t, X_i),$$

and as a result of the symmetry property of the integrand the validity of the following equality

$$\begin{aligned} & \sum_{Z \subset X \setminus Y} \mathfrak{A}_{1+|Z|}(-t, \{Y\}, Z) \sum_{P: X \setminus Y \setminus Z = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(-t, X_i) = \\ & = \sum_{k=0}^n \sum_{i_1 < \dots < i_k=1}^n \mathfrak{A}_{1+k}(-t, \{Y\}, x_{s+1}, \dots, x_{s+k}) \sum_{P: (x_{s+k+1}, \dots, x_{s+n}) = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(-t, X_i), \end{aligned}$$

we have

$$\begin{aligned} (e^a S(-t) D(0), u) &= \sum_{s=0}^{\infty} \frac{1}{s!} \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int \mathfrak{A}_{1+|X \setminus Y|}(-t, \{Y\}, X \setminus Y) \sum_{k=0}^{\infty} \frac{1}{k!} \times \\ & \times \sum_{P: (x_{s+n+1}, \dots, x_{s+n+k}) = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(-t, X_i) D_{s+n+k}(0) \prod_{i=1}^s u(x_i) dx_1 \dots dx_{s+n+k}. \end{aligned}$$

Here the solution of cluster expansions (17)

$$\mathfrak{A}_{1+n}(-t, \{Y\}, X \setminus Y) = \sum_{P: (\{Y\}, X \setminus Y) = \bigcup_i X_i} (-1)^{|P|-1} (|P| - 1)! \prod_{X_i \subset P} S_{|\theta(X_i)|}(-t, \theta(X_i)) \quad (18)$$

is the  $(1+n)$ th-order cumulant of groups of operators (16), and we introduced the declusterization mapping by the following formula:  $\theta(\{Y\}, X \setminus Y) = X$ .

According to the validity of the equality

$$\begin{aligned} & \int \dots \int \sum_{P: (x_{s+n+1}, \dots, x_{s+n+k}) = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(-t, X_i) D_{s+n+k}(0) dx_{s+n+1} \dots dx_{s+n+k} = \\ & = \int \dots \int D_{s+n+k}(0) dx_{s+n+1} \dots dx_{s+n+k}, \end{aligned}$$

and the similar equality for the normalizing factor [13]

$$(S(-t) D(0), I) = (D(0), I),$$

and taking into account the definition of initial marginal distribution functions, from relation (7) we derive

$$F_s(t, Y) = \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int \mathfrak{A}_{1+n}(-t, \{Y\}, X \setminus Y) F_{s+n}(0, X) dx_{s+1} \dots dx_{s+n}, \quad (19)$$

where  $\mathfrak{A}_{1+n}(-t, \{Y\}, X \setminus Y)$  is  $(1+n)$ th-order cumulant (18).

In fact the following criterion is valid. Expansion (19) is a solution of the initial-value problem of the BBGKY hierarchy (15) if and only if the evolution operators  $\mathfrak{A}_{1+n}(-t)$ ,  $n \geq 0$ , satisfy the recurrence relations (17).

We indicate that nonperturbative solution (19) of the BBGKY hierarchy is transformed to the form of the perturbation (iteration) series as a result of applying of analogs of the Duhamel equation to cumulants (18) of groups of operators [14, 15].

For the first time a nonperturbative solution of the BBGKY hierarchy was constructed in paper [8] (see also [13]) in the form of an expansion over particle clusters which evolution is governed by the corresponding-order reduced cumulant of groups of operators (16)

$$U_{1+n}(-t, \{Y\}, X \setminus Y) = \sum_{k=0}^n (-1)^k \frac{n!}{k!(n-k)!} S_{s+n-k}(-t, Y, x_{s+1}, \dots, x_{s+n-k}). \quad (20)$$

Indeed, using the reduced cluster expansions of operators (16) over reduced cumulants

$$S_{s+n}(-t, Y, X \setminus Y) = \sum_{k=0}^n \frac{n!}{k!(n-k)!} U_{1+k}(-t, \{Y\}, x_{s+1}, \dots, x_{s+k}),$$

for the generating functional  $(\tilde{D}(t), u+1)$  we have as above

$$\begin{aligned} (\tilde{D}(t), u+1) &= (D(0), I)^{-1} (S(-t)D(0), u+1) = \\ &= (D(0), I)^{-1} \sum_{s=0}^{\infty} \frac{1}{s!} \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int U_{1+n}(-t) \sum_{k=0}^{\infty} \frac{1}{k!} D_{s+n+k}(0) \prod_{i=1}^s u(x_i) dx_1 \dots dx_{s+n+k}, \end{aligned}$$

and thus,

$$F_s(t, Y) = \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int U_{1+n}(-t, \{Y\}, X \setminus Y) F_{s+n}(0, X) dx_{s+1} \dots dx_{s+n},$$

where  $U_{1+n}(-t)$  is the  $(1+n)$ th-order reduced cumulant (20).

### 3 Evolution equations in functional derivatives for correlations

#### 3.1 The Liouville hierarchy for correlation functions

In addition to an approach of the description of the evolution of states of many-particle systems in terms of distribution functions one more an equivalent approach is given by means of correlation functions which governed by the Liouville hierarchy.

We introduce the generating functional  $(g(t), u)$  of correlation functions  $g_s(t, x_1, \dots, x_s)$ ,  $s \geq 1$ , by means of generating functional (4) as follows

$$(D(t), u) = e^{(g(t), u)}. \quad (21)$$



Then taking into account the equality for  $k \geq 1$

$$\frac{\delta^k}{\delta u(x_1) \dots \delta u(x_k)}(D(t), u) = e^{(g, u)} \sum_{\substack{P: (x_1, \dots, x_k) = \bigcup_j X_j, \\ X_j \equiv (x_{i_1}, \dots, x_{i_{|X_j|}})}} \prod_{X_j \subset P} \frac{\delta^{|X_j|}}{\delta u(x_{i_1}) \dots \delta u(x_{i_{|X_j|}})}(g(t), u),$$

according to the Liouville equation in functional derivatives (5), the evolution of states of many-particle systems in terms of generating functional (21) of correlation functions is governed by the following evolution equation in functional derivatives

$$\begin{aligned} \frac{d}{dt}(g(t), u) &= \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)}(g(t), u) \right\} u(x_1) dx_1 + \\ &+ \frac{1}{2!} \int \int \left\{ \Phi(q_1 - q_2), \left( \frac{\delta^2}{\delta u(x_1) \delta u(x_2)}(g(t), u) + \prod_{j=1}^2 \frac{\delta}{\delta u(x_j)}(g(t), u) \right) \right\} u(x_1) u(x_2) dx_1 dx_2, \end{aligned} \quad (22)$$

or in case of the Hamiltonian (12) this equation has the form

$$\begin{aligned} \frac{d}{dt}(g(t), u) &= \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)}(g(t), u) \right\} u(x_1) dx_1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int \dots \int \left\{ \Phi^{(n)}(q_1, \dots, q_n), \right. \\ &\left. \sum_{\substack{P: (x_1, \dots, x_n) = \bigcup_j X_j, \\ X_j \equiv (x_{i_1}, \dots, x_{i_{|X_j|}})}} \prod_{X_j \subset P} \frac{\delta^{|X_j|}}{\delta u(x_{i_1}) \dots \delta u(x_{i_{|X_j|}})}(g(t), u) \right\} \prod_{i=1}^n u(x_i) dx_1 \dots dx_n, \end{aligned} \quad (23)$$

where  $\sum_{P: (x_1, \dots, x_n) = \bigcup_j X_j}$  is the sum over all possible partitions  $P$  of the set  $(x_1, \dots, x_n)$  into  $|P|$  nonempty mutually disjoint subsets  $X_j \equiv (x_{i_1}, \dots, x_{i_{|X_j|}}) \subset (x_1, \dots, x_n)$ .

Taking into account equality (2), we observe that the correlation functions  $g_s(t)$ ,  $s \geq 1$ , are determined by the Liouville hierarchy [16, 17]

$$\begin{aligned} \frac{\partial}{\partial t} g_s(t, Y) &= \{H_s, g_s(t, Y)\} + \\ &+ \sum_{\substack{P: Y = \bigcup_i X_i, \\ |P| > 1}} \sum_{\substack{Z_1 \subset X_1, \\ Z_1 \neq \emptyset}} \dots \sum_{\substack{Z_{|P|} \subset X_{|P|}, \\ Z_{|P|} \neq \emptyset}} \left\{ \Phi^{(\sum_{r=1}^{|P|} |Z_r|)}(Z_1, \dots, Z_{|P|}), \prod_{X_i \subset P} g_{|X_i|}(t, X_i) \right\}, \end{aligned} \quad (24)$$

where notations accepted above are used.

We note that the correlation functions  $g_n(t)$ ,  $n \geq 1$ , are interpreted as the functions that describe correlations of states  $D_n(t)$ ,  $n \geq 1$ , governed by the Liouville equations (6). Indeed, according to definition (2), from relation (21) for generating functionals we obtain the cluster expansions of distribution functions over the correlation functions

$$D_s(t, Y) = \sum_{P: Y = \bigcup_i X_i} \prod_{X_i \subset P} g_{|X_i|}(t, X_i), \quad s \geq 1, \quad (25)$$

i.e. the correlation functions are the cumulants (semi-invariants) of distribution functions

$$g_s(t, Y) = \sum_{P: Y = \bigcup_i X_i} (-1)^{|P|-1} (|P| - 1)! \prod_{X_i \subset P} D_{|X_i|}(t, X_i), \quad s \geq 1.$$

The validity of relations (25) is a consequence of the following equality

$$e^{(g(t), u)} = (\mathbb{E} \exp_* g(t), u), \quad (26)$$

where we denote by  $(\mathbb{E} \exp_* g(t), u)$  the generating functional of the sequence of functions

$$(\mathbb{E} \exp_* g(t))_s(Y) = \sum_{P: Y = \bigcup_i X_i} \prod_{X_i \subset P} g_{|X_i|}(t, X_i), \quad s \geq 1.$$

Indeed, on sequences of functions  $f, \tilde{f} \in L^1$  we define the  $*$ -product

$$(f * \tilde{f})_{|Y|}(Y) = \sum_{Z \subset Y} f_{|Z|}(Z) \tilde{f}_{|Y \setminus Z|}(Y \setminus Z), \quad (27)$$

where  $\sum_{Z \subset Y}$  is the sum over all subsets  $Z$  of the set  $Y \equiv (x_1, \dots, x_s)$ . By means of definition (27) of the  $*$ -product we introduce on sequences  $f = (0, f_1(x_1), \dots, f_n(x_1, \dots, x_n), \dots)$  the mapping  $\mathbb{E} \exp_*$  by the expansions

$$\begin{aligned} (\mathbb{E} \exp_* f)_{|Y|}(Y) &= (\mathbb{I} + \sum_{n=1}^{\infty} \frac{1}{n!} f^{*n})_{|Y|}(Y) = \\ &= 1\delta_{|Y|,0} + \sum_{P: Y = \bigcup_i X_i} \prod_{X_i \subset P} f_{|X_i|}(X_i), \end{aligned} \quad (28)$$

where we use the notations accepted above,  $\delta_{|Y|,0}$  is a Kronecker symbol and  $\mathbb{I} \equiv (1, 0, \dots, 0, \dots)$ . Then observing the validity of the equality

$$(f * \tilde{f}, u) = (f, u)(\tilde{f}, u), \quad (29)$$

in view of (28) we justify equality (26).

A solution of the Cauchy problem of the Liouville hierarchy (24) for the initial data  $g(0)$  is defined by the following evolution operator [16]

$$g_s(t, Y) = \mathcal{S}(t, Y|g(0)) \equiv \sum_{P: Y = \bigcup_i X_i} \mathfrak{A}_{|P|}(-t, \{X_1\}, \dots, \{X_{|P|}\}) \prod_{X_i \subset P} g_{|X_i|}(0, X_i). \quad (30)$$

Here  $\mathfrak{A}_{|P|}(-t)$  is the  $|P|$ th-order cumulant of groups of operators (16) given by the expansion

$$\begin{aligned} \mathfrak{A}_{|P|}(-t, \{X_1\}, \dots, \{X_{|P|}\}) &\doteq \\ &\doteq \sum_{P': (\{X_1\}, \dots, \{X_{|P|}\}) = \bigcup_k Z_k} (-1)^{|P'|-1} (|P'| - 1)! \prod_{Z_k \subset P'} S_{|\theta(Z_k)|}(-t, \theta(Z_k)), \end{aligned} \quad (31)$$

where  $\sum_{P': (\{X_1\}, \dots, \{X_{|P|}\}) = \bigcup_k Z_k}$  is the sum over all possible partitions  $P'$  of the set  $(\{X_1\}, \dots, \{X_{|P|}\})$  into  $|P'|$  nonempty mutually disjoint subsets  $Z_k \subset (\{X_1\}, \dots, \{X_{|P|}\})$ .

Really, taking into account formula (16) for the solution of the Liouville equations and the cluster expansions of distribution functions over correlation functions at initial time:  $D(0) = \mathbb{E}xp_*g(0)$ , from equality (26) we obtain

$$(g(t), u) = (\mathbb{L}n_*(\mathbb{I} + S(-t)\mathbb{E}xp_*g(0)), u),$$

where the inverse mapping  $\mathbb{L}n_*$  to mapping (28) is defined by

$$\begin{aligned} (\mathbb{L}n_*(\mathbb{I} + f))_{|Y|}(Y) &= \left( \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} f^{*n} \right)_{|Y|}(Y) = \\ &= \sum_{P: Y = \bigcup_i X_i} (-1)^{|P|-1} (|P| - 1)! \prod_{X_i \subset P} f_{|X_i|}(X_i). \end{aligned}$$

As a result of regrouping terms with respect to the same initial data we derive formula (30) in componentwise form.

### 3.2 Some relations between generating functionals

Starting from an alternative approach to the description of states by the generating functional of correlation functions (21), we define the generating functional of marginal distribution functions by means of such generating functional. Moreover we introduce also the generating functional of the marginal correlation functions and consider relations of these generating functionals.

According to relations (7) and (21), the generating functional of marginal distribution functions is determined by means of generating functional of correlation functions as follows

$$(F(t), u) = e^{(g(t), u+1) - (g(t), I)}. \quad (32)$$

Using this relation, the BBGKY hierarchy in functional derivatives (14) can be derived on the basis of the Liouville hierarchy in functional derivatives (22).

From (32) in view of definition (2) we obtain the expression for marginal distribution functions in terms of correlation functions

$$F_s(t, Y) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int g_{1+n}(t, \{Y\}, x_{s+1}, \dots, x_{s+n}) dx_{s+1} \dots dx_{s+n}, \quad s \geq 1, \quad (33)$$

where we denote by  $(\{Y\})$  the set consisting of one element  $Y = (1, \dots, s)$ , and the correlation functions  $g_{1+n}(t, \{Y\}, x_{s+1}, \dots, x_{s+n})$ ,  $n \geq 0$ , are solutions of the Liouville hierarchy (24) in case of particle cluster of  $s$  particles and particles [18]. To prove relation (33) we transform the functional from the right-hand side of relation (32) to the canonical form using equalities (26) and (8)

$$\begin{aligned} e^{(g(t), u+1) - (g(t), I)} &= (\mathbb{E}xp_*g(t), I)^{-1} (\mathbb{E}xp_*g(t), u+1) = \\ &= (\mathbb{E}xp_*g(t), I)^{-1} (e^a \mathbb{E}xp_*g(t), u). \end{aligned}$$

The last functional is the generating functional of the sequence of functions

$$(\mathbb{E}xp_*g(t), I)^{-1} e^a \mathbb{E}xp_*g(t).$$

To write down it in the component-wise form on measurable functions we introduce the following mappings

$$\begin{aligned} (\mathfrak{d}_Y f)_n &\doteq f_{|Y|+n}(Y, x_{s+1}, \dots, x_{s+n}), \\ (\mathfrak{d}_{\{Y\}} f)_n &\doteq f_{1+n}(\{Y\}, x_{s+1}, \dots, x_{s+n}), \quad n \geq 0. \end{aligned}$$

Then we have

$$(\mathbb{E}xp_*g(t), I)^{-1} (e^a \mathbb{E}xp_*g(t))_s(Y) = (\mathbb{E}xp_*g(t), I)^{-1} (\mathfrak{d}_Y \mathbb{E}xp_*g(t), I).$$

Owing the validity of the following equalities [18]

$$\mathfrak{d}_Y \mathbb{E}xp_*g(t) = \mathfrak{d}_{\{Y\}} \mathbb{E}xp_*g(t),$$

and

$$\mathfrak{d}_{\{Y\}} \mathbb{E}xp_*g(t) = \mathbb{E}xp_*g(t) * \mathfrak{d}_{\{Y\}} g(t),$$

and according to equality (29), we finally derive (33)

$$(\mathbb{E}xp_*g(t), I)^{-1} (\mathfrak{d}_Y \mathbb{E}xp_*g(t), I) = (\mathfrak{d}_{\{Y\}} g(t), I).$$

On the basis of solution (30) of the Liouville hierarchy (22) and relation (32) for generating functionals, we also derive nonperturbative solution (19) of initial-value problem of the BBGKY hierarchy (11).

By analogy with relation (7) we introduce the generating functional of the marginal correlation functions by means of generating functional of correlation functions as follows

$$(G(t), u) = (g(t), u+1) - (g(t), I), \quad (34)$$

or in view of definition (2) in componentwise form it has the form

$$G_s(t, x_1, \dots, x_s) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int g_{s+n}(t, x_1, \dots, x_{s+n}) dx_{s+1} \dots dx_{s+n}, \quad s \geq 1, \quad (35)$$

where the correlation functions  $g_{s+n}(t)$  are solutions of the Liouville hierarchy (24). We emphasize that every term of marginal correlation function expansion (35) is determined by the  $(s+n)$ th-particle correlation function as contrasted to marginal distribution function expansion (33) which is defined by the  $(1+n)$ th-particle correlation function.

From relations (34) and (32) we obtain the relation of the generating functionals of marginal distribution functions and marginal correlation functions

$$(F(t), u) = e^{(G(t), u)}. \quad (36)$$

We note that in view of definition (2) in componentwise form relation (36) is the cluster expansions of the marginal distribution functions over the marginal correlation functions (it is an analog of cluster expansions (25) or (21))

$$F_s(t, Y) = \sum_{P: Y = \bigcup_i X_i} \prod_{X_i \subset P} G_{|X_i|}(t, X_i), \quad s \geq 1,$$

where  $\sum_{P: Y = \bigcup_i X_i}$  is the sum over all possible partitions  $P$  of the set  $Y \equiv (x_1, \dots, x_s)$  into  $|P|$  nonempty mutually disjoint subsets  $X_i \subset Y$ .

### 3.3 The nonlinear BBGKY hierarchy in functional derivatives

From relation (34) we derive the nonlinear BBGKY hierarchy in functional derivatives for the generating functional of marginal correlation functions on the basis of the Liouville hierarchy in functional derivatives (22)

$$\begin{aligned} \frac{d}{dt}(G(t), u) &= \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)} \right\} (G(t), u) (u(x_1) + 1) dx_1 + \\ &+ \frac{1}{2!} \int \int \left\{ \Phi(q_1 - q_2), \left( \frac{\delta^2}{\delta u(x_1) \delta u(x_2)} (G(t), u) + \prod_{j=1}^2 \frac{\delta}{\delta u(x_j)} (G(t), u) \right) \right\} \prod_{i=1}^2 (u(x_i) + 1) dx_1 dx_2, \end{aligned} \quad (37)$$

or in case of the Hamiltonian (12) this equation has the form

$$\begin{aligned} \frac{d}{dt}(G(t), u) &= \int \left\{ K(p_1), \frac{\delta}{\delta u(x_1)} (G(t), u) \right\} (u(x_1) + 1) dx_1 + \\ &+ \sum_{n=1}^{\infty} \frac{1}{n!} \int \dots \int \left\{ \Phi^{(n)}(q_1, \dots, q_n), \sum_{\substack{P: (x_1, \dots, x_n) = \bigcup_j X_j, \\ X_j \equiv (x_{i_1}, \dots, x_{i_{|X_j|}})}} \prod_{X_j \subset P} \frac{\delta^{|X_j|} (G(t), u)}{\delta u(x_{i_1}) \dots \delta u(x_{i_{|X_j|}})} \right\} \times \\ &\times \prod_{i=1}^n (u(x_i) + 1) dx_1 \dots dx_n, \end{aligned} \quad (38)$$

where we use notations accepted above in equation (23).

Taking into account equality (2), we observe that the marginal correlation functions are determined by the nonlinear BBGKY hierarchy

$$\begin{aligned} \frac{\partial}{\partial t} G_s(t, Y) &= \{H_s, G_s(t, Y)\} + \\ &+ \sum_{\substack{P: Y = \bigcup_i X_i, \\ |P| > 1}} \sum_{\substack{Z_1 \subset X_1, \\ Z_1 \neq \emptyset}} \dots \sum_{\substack{Z_{|P|} \subset X_{|P|}, \\ Z_{|P|} \neq \emptyset}} \left\{ \Phi^{(\sum_{r=1}^{|P|} |Z_r|)}(Z_1, \dots, Z_{|P|}), \prod_{X_i \subset P} G_{|X_i|}(t, X_i) \right\} + \\ &+ \sum_{n=1}^{\infty} \sum_{k=1}^n \sum_{s=1}^s \int \dots \int \left\{ \Phi^{(n+1)}(q_{j_1}, \dots, q_{j_k}, q_{s+1}, \dots, q_{s+n+1-k}), \right. \\ &\quad \left. \sum_{\substack{P: (x_1, \dots, x_{s+n+1-k}) = \bigcup_j X_j, |P| \leq n+1, \\ X_j \not\subseteq Y \setminus (x_{j_1}, \dots, x_{j_k})}} \prod_{X_j \subset P} G_{|X_j|}(t, X_j) \right\} dx_{s+1} \dots dx_{s+n+1-k}. \end{aligned} \quad (39)$$

We can see that the structure of the Liouville hierarchy (22) and the nonlinear BBGKY hierarchy (37) in functional derivatives is similar in contrast to the structure of these hierarchies for corresponding correlation functions.

On the basis of solution (30) of the Liouville hierarchy (24) and relation (34) for generating functionals, as above in case of relation (7) we derive a nonperturbative solution of initial-value problem of the nonlinear BBGKY hierarchy (39).

Taking into account the equality

$$(g(t), u + 1) = (\mathcal{S}(t|g(0)), u + 1) = (e^a \mathcal{S}(t|g(0)), u), \quad (40)$$

in the functional  $(e^a \mathcal{S}(t|g(0)), u)$  we expand operators (30) over the corresponding cumulants. As a result from relation (34) we derive a solution expansion of the nonlinear BBGKY hierarchy [19]

$$G_s(t, Y) = \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int U_{1+n}(t; \{Y\}, x_{s+1}, \dots, x_{s+n} | G(0)) dx_{s+1} \dots dx_{s+n}, \quad s \geq 1, \quad (41)$$

where the  $(n + 1)th$ -order reduced cumulant  $U_{1+n}(t)$  of groups (30) has been introduced

$$\begin{aligned} U_{1+n}(t; \{Y\}, x_{s+1}, \dots, x_{s+n} | G(0)) &\doteq \sum_{k=0}^n (-1)^k \frac{n!}{k!(n-k)!} \times \\ &\times \sum_{P: (x_1, \dots, x_{s+n-k}) = \bigcup_i X_i} \mathfrak{A}_{|P|}(-t, X_1, \dots, X_{|P|}) \sum_{k_1=0}^k \frac{k!}{k_1!(k-k_1)!} \dots \sum_{k_{|P|-1}=0}^k \frac{k_{|P|-2}!}{k_{|P|-1}!(k_{|P|-2}-k_{|P|-1})!} \\ &\times G_{|X_1|+k-k_1}(0, X_1, x_{s+n-k+1}, \dots, x_{s+n-k_1}) \dots G_{|X_{|P|}|+k_{|P|-1}}(0, X_{|P|}, x_{s+n-k_{|P|-1}+1}, \dots, x_{s+n}), \end{aligned} \quad (42)$$

and  $\mathfrak{A}_{|P|}(-t)$  is the  $|P|th$ -order cumulant defined by the formula (31).

We give simplest examples of reduced nonlinear cumulants (42):

$$\begin{aligned} U_1(t; \{Y\} | G(0)) &= \mathcal{G}(t; Y | G(0)) = \\ &= \sum_{P: Y = \bigcup_i X_i} \mathfrak{A}_{|P|}(-t, \{X_1\}, \dots, \{X_{|P|}\}) \prod_{X_i \subset P} G_{|X_i|}(0, X_i), \\ U_2(t; \{Y\}, x_{s+1} | G(0)) &= \sum_{P: (Y, x_{s+1}) = \bigcup_i X_i} \mathfrak{A}_{|P|}(-t, \{X_1\}, \dots, \{X_{|P|}\}) \prod_{X_i \subset P} G_{|X_i|}(0, X_i) - \\ &- \sum_{P: Y = \bigcup_i X_i} \mathfrak{A}_{|P|}(-t, \{X_1\}, \dots, \{X_{|P|}\}) \sum_{j=1}^{|P|} \prod_{\substack{X_i \subset P, \\ X_i \neq X_j}} G_{|X_i|}(0, X_i) G_{|X_j|+1}(0, X_j, x_{s+1}). \end{aligned}$$

In case of initial data satisfying a chaos property, i.e.  $G^{(1)}(0) \equiv (0, G_1(0, 1), 0, \dots)$ , for the  $(1 + n)th$ -order reduced cumulant (42) we have

$$U_{1+n}(t; \{Y\}, X \setminus Y | G^{(1)}(0)) = \mathfrak{A}_{s+n}(-t, X) \prod_{i=1}^{s+n} G_1(0, x_i),$$

where  $\mathfrak{A}_{s+n}(-t)$  is  $(s + n)th$ -order cumulant (18), and solution expansion (41) takes the more transparent structure. From the structure of this series it is clear that in case of absence of correlations at initial time the correlations generated by the dynamics of many-particle systems are completely governed by cumulants (18) of groups of operators (16).

## 4 The dual BBGKY hierarchy in functional derivatives

### 4.1 A generating functional of marginal observables

The evolution of many-particle systems is described within the framework of the evolution of states or in terms of an equivalent approach as the evolution of observables [13]. The evolution of observables of a system of a non-fixed number of particles is described by the sequences  $A(t) = (A_0, A_1(t, x_1), \dots, A_n(t, x_1, \dots, x_n), \dots)$  of observables. The bounded function  $A_n(t, x_1, \dots, x_n)$  is defined on the  $n$ -particle phase space and symmetric with respect to the permutations of arguments  $x_1, \dots, x_s$ . According to definition (1) we introduce the generating functional  $(A(t), u)$  of observables by the expansion

$$(A(t), u) \doteq \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int A_n(t, x_1, \dots, x_n) \prod_{i=1}^n u(x_i) dx_1 \dots dx_n. \quad (43)$$

For the integrable functions  $u(x_i)$ ,  $i \geq 1$ , functional (43) exists.

Within the framework of generating functional (43) the evolution of observables of many-particle systems with the Hamiltonian (3) is governed by the following evolution equation in functional derivatives

$$\begin{aligned} \frac{d}{dt}(A(t), u) &= \int \left\{ \frac{\delta}{\delta u(x_1)} (A(t), u), K(p_1) \right\} u(x_1) dx_1 + \\ &+ \frac{1}{2!} \int \int \left\{ \frac{\delta^2}{\delta u(x_1) \delta u(x_2)} (A(t), u), \Phi(q_1 - q_2) \right\} u(x_1) u(x_2) dx_1 dx_2, \end{aligned} \quad (44)$$

where  $\{.,.\}$  is the Poisson bracket. Taking into account equality (2), we establish that observables  $A_n(t)$ ,  $n \geq 1$ , are determined by the sequence of the Liouville equations for observables

$$\frac{\partial}{\partial t} A_n(t) = \{A_n(t), H_n\}, \quad n \geq 1, \quad (45)$$

or vice versa the generating functional of solutions of the Liouville equations (45) satisfies equation (44).

We introduce a generating functional of marginal observables  $B(t) = (B_0, B_1(t, x_1), \dots, B_s(t, x_1, \dots, x_s), \dots)$  by means of generating functional (43) as follows

$$(B(t), u) = (A(t), u e^{-\int u(x) dx}), \quad (46)$$

where we use the notation

$$u e^{-\int u(x) dx} = (1, u(x_1), \dots, \prod_{i=1}^n u(x_i), \dots) \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int \dots \int \prod_{j=1}^k u(x_j) dx_1 \dots dx_k.$$

A generating functional of marginal observables gives an equivalent approach to the description of the evolution of finitely many particles in addition to generating functional of observables (43) and it is adopted for the description of infinite-particle systems.

In consequence of introduced relation (46) we establish the relation between marginal observables and observables. We transform generating functional  $(A(t), ue^{-\int u(x)dx})$  to form (1), and thus, we determine functions generated by this functional. The following equality holds (the dual analog of equality (8))

$$(A(t), ue^{-\int u(x)dx}) = (e^{-\mathfrak{a}^+} A(t), u), \quad (47)$$

where on  $b \in L^\infty$  the operator  $\mathfrak{a}^+$  is defined by the formula (an analog of the creation operator [13], which is an adjoint operator to operator (9) in the sense of mean value functional [13])

$$(\mathfrak{a}^+ b)_s(x_1, \dots, x_s) \doteq \sum_{j=1}^s b_{s-1}((x_1, \dots, x_s) \setminus (x_j)).$$

Indeed we have

$$\begin{aligned} (A(t), ue^{-\int u(x)dx}) &= \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int \dots \int A_n(t, x_1, \dots, x_n) \prod_{i=1}^{k+n} u(x_i) dx_1 \dots dx_{k+n} = \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int \sum_{k=0}^n (-1)^k \frac{n!}{k!(n-k)!} A_{n-k}(t, x_1, \dots, x_{n-k}) \prod_{i=1}^n u(x_i) dx_1 \dots dx_n, \end{aligned}$$

and therefore in view of symmetry property of observables, according to definition (2), from relation (46) we obtain the expression for marginal ( $s$ -particle) observables within the framework of nonequilibrium grand canonical ensemble [20]

$$B_s(t, x_1, \dots, x_s) = \sum_{n=0}^s \frac{(-1)^n}{n!} \sum_{j_1 \neq \dots \neq j_n=1}^s A_{s-n}(t, (x_1, \dots, x_s) \setminus (x_{j_1}, \dots, x_{j_n})). \quad (48)$$

Using relation (46), from the Liouville equation in functional derivatives for observables (44), we derive the evolution equation for the generating functional of marginal observables

$$\begin{aligned} \frac{d}{dt}(B(t), u) &= \int \left\{ \frac{\delta}{\delta u(x_1)} (B(t), u), K(p_1) \right\} u(x_1) dx_1 + \\ &+ \frac{1}{2!} \int \int \left\{ \frac{\delta^2}{\delta u(x_1) \delta u(x_2)} (B(t), u) + \sum_{j=1}^2 \frac{\delta}{\delta u(x_j)} (B(t), u), \Phi(q_1 - q_2) \right\} \prod_{i=1}^2 u(x_i) dx_1 dx_2. \end{aligned} \quad (49)$$

We are referred to this evolution equation as the dual BBGKY hierarchy in functional derivatives. Taking into account equality (2), from evolution equation (49) we establish that the marginal observables  $B_s(t)$ ,  $s \geq 1$ , are determined by the dual BBGKY hierarchy [20, 21]

$$\frac{\partial}{\partial t} B_s(t, Y) = \{B_s(t, Y), H_s\} + \sum_{i \neq j=1}^s \{B_{s-1}(t, Y \setminus (x_i)), \Phi(q_i - q_j)\}, \quad s \geq 1, \quad (50)$$

where  $Y \equiv (x_1, \dots, x_s)$  and  $Y \setminus (x_i) \equiv (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_s)$ . As above in case of the Liouville equations (45) the generating functional of solutions of the dual BBGKY hierarchy (50) satisfies equation (49).



To clarify the structure of stated above evolution equations in functional derivatives we generalize them for a system of particles interacting via many-body interaction potentials. In this case the Liouville equation in functional derivatives has the form

$$\begin{aligned} \frac{d}{dt}(A(t), u) &= \int \left\{ \frac{\delta}{\delta u(x_1)}(A(t), u), K(p_1) \right\} u(x_1) dx_1 + \\ &+ \sum_{n=1}^{\infty} \frac{1}{n!} \int \cdots \int \left\{ \frac{\delta^n}{\delta u(x_1) \cdots \delta u(x_n)}(A(t), u), \Phi^{(n)}(q_1, \dots, q_n) \right\} \prod_{i=1}^n u(x_i) dx_1 \cdots dx_n, \end{aligned} \quad (51)$$

and observables are determined by a sequence of the Liouville equations (45) with the Hamiltonian (12) respectively. The dual BBGKY hierarchy in functional derivatives for the generating functional of marginal observables takes the form

$$\begin{aligned} \frac{d}{dt}(B(t), u) &= \int \left\{ \frac{\delta}{\delta u(x_1)}(B(t), u), K(p_1) \right\} u(x_1) dx_1 + \sum_{n=1}^{\infty} \frac{1}{n!} \times \\ &\times \int \cdots \int \left\{ \sum_{k=1}^n \sum_{i_1 < \dots < i_k=1}^n \frac{\delta^k}{\delta u(x_{i_1}) \cdots \delta u(x_{i_k})}(B(t), u), \Phi^{(n)}(q_1, \dots, q_n) \right\} \prod_{i=1}^n u(x_i) dx_1 \cdots dx_n, \end{aligned} \quad (52)$$

and the marginal observables are governed by the dual BBGKY hierarchy [21]

$$\begin{aligned} \frac{\partial}{\partial t} B_s(t, Y) &= \{B_s(t, Y), H_s\} + \\ &+ \sum_{n=1}^s \frac{1}{n!} \sum_{k=n+1}^s \frac{1}{(k-n)!} \sum_{j_1 \neq \dots \neq j_k=1}^s \{B_{s-n}(t, Y \setminus (x_{j_1}, \dots, x_{j_n})), \Phi^{(k)}(x_{j_1}, \dots, x_{j_k})\}. \end{aligned} \quad (53)$$

As is obvious the evolution equations in functional derivatives for dual generating functionals (4),(43) have the form (13),(51) and correspondingly for dual generating functionals (7),(46) the hierarchies in functional derivatives have the form (14),(52).

## 4.2 A nonperturbative solution of the dual BBGKY hierarchy

On the basis of a solution of the Liouville equation (45) and relation (46) for generating functionals, we construct a nonperturbative solution of the Cauchy problem of the dual BBGKY hierarchy (53). With this aim we consider the sequence

$$A(t) = (A_0, S_1(t)A_1(0, x_1), \dots, S_n(t)A_n(0, x_1, \dots, x_n), \dots),$$

where the evolution operator  $S_n(t)$  is defined on the space  $L_n^\infty$  by formula (16), and it is determined a solution of the Cauchy problem of the Liouville equation for observables of the  $n$ -particle system with the initial data  $A_n(0)$ . Using equality (47), in the functional  $(e^{-a^+} S(t)A(0), u)$  we expand operators  $S_n(t)$ ,  $n \geq 1$ , over their cumulants as the following cluster expansions

$$\begin{aligned} (-1)^n S_{s-n}(t, Y \setminus X) &= \\ &= \sum_{k=0}^n (-1)^{n-k} \sum_{i_1 < \dots < i_k \in (j_1, \dots, j_n)} \mathfrak{A}_{1+k}(t, \{Y \setminus (x_{i_1}, \dots, x_{i_k})\}, x_{i_1}, \dots, x_{i_k}), \end{aligned} \quad (54)$$

where the abridged notations are introduced:  $X \equiv (x_{j_1}, \dots, x_{j_n}) \subset Y$ ,  $(x_{i_1}, \dots, x_{i_k}) \subset X$ . Then the following equalities are true

$$\begin{aligned}
 (e^{-\mathfrak{a}^+} S(t) A(0), u) &= \\
 &= \sum_{s=0}^{\infty} \frac{1}{s!} \int \dots \int \sum_{n=0}^s \frac{(-1)^n}{n!} \sum_{j_1 \neq \dots \neq j_n=1}^s S_{s-n}(t) A_{s-n}(0)(Y \setminus X) \prod_{i=1}^s u(x_i) dx_1 \dots dx_s = \\
 &= \sum_{s=0}^{\infty} \frac{1}{s!} \int \dots \int \sum_{n=0}^s \frac{1}{n!} \sum_{j_1 \neq \dots \neq j_n=1}^s \mathfrak{A}_{1+n}(t, \{Y \setminus (x_{j_1}, \dots, x_{j_n})\}, x_{j_1}, \dots, x_{j_n}) \times \\
 &\times \sum_{k=0}^{s-n} \frac{(-1)^k}{k!} \sum_{\substack{i_1 \neq \dots \neq i_k=1, \\ i_1, \dots, i_k \neq j_1, \dots, j_n}}^s A_{s-n-k}(0, Y \setminus X \setminus (x_{i_1}, \dots, x_{i_k})) \prod_{i=1}^s u(x_i) dx_1 \dots dx_s.
 \end{aligned}$$

Owing to the definition of initial marginal observables (48), from relation (46) and equality (47) we finally derive

$$B_s(t, Y) = \sum_{n=0}^s \frac{1}{n!} \sum_{j_1 \neq \dots \neq j_n=1}^s \mathfrak{A}_{1+n}(t, \{Y \setminus X\}, X) B_{s-n}(0, Y \setminus X), \quad (55)$$

where  $X \equiv (x_{j_1}, \dots, x_{j_n}) \subset Y$  and the  $(1+n)th$ -order cumulant of groups of operators (16) is defined as follows [15], [21]

$$\mathfrak{A}_{1+n}(t, \{Y \setminus X\}, X) \doteq \sum_{P: \{Y \setminus X\}, X = \bigcup_i X_i} (-1)^{|P|-1} (|P| - 1)! \prod_{X_i \subset P} S_{|\theta(X_i)|}(t, \theta(X_i)), \quad (56)$$

and we use notations accepted above, for example,

$$\begin{aligned}
 \mathfrak{A}_1(t, \{Y\}) &= S_s(t, Y), \\
 \mathfrak{A}_2(t, \{Y \setminus (x_j)\}, x_j) &= S_s(t, Y) - S_{s-1}(t, Y \setminus (x_j)) S_1(t, x_j).
 \end{aligned}$$

To prove that cumulants (56) are solutions of recurrence relations (54) we observe that recurrence relations (54) hold on functions  $b_{s-n}(Y \setminus X)$ , and thus, the following identity is true

$$\begin{aligned}
 &(-1)^n S_{s-n}(t, Y \setminus X) \sum_{P: X = \bigcup_i X_i} (-1)^{|P|} |P|! \prod_{X_i \subset P} S_{|X_i|}(t, X_i) b_{s-n}(Y \setminus X) = \\
 &= \sum_{k=0}^n (-1)^{n-k} \sum_{i_1 < \dots < i_k \in (j_1, \dots, j_n)} \mathfrak{A}_{1+k}(t, \{Y \setminus (x_{i_1}, \dots, x_{i_k})\}, x_{i_1}, \dots, x_{i_k}) b_{s-n}(Y \setminus X),
 \end{aligned}$$

where  $\sum_{P: X = \bigcup_i X_i}$  is the sum over all possible partitions  $P$  of the set  $X$  into  $|P|$  nonempty mutually disjoint subsets  $X_i \subset X$ . These recurrence relations are rearranged form of the cluster expansions of the evolution operators  $S_s(t)$ ,  $s \geq 1$ ,

$$S_s(t, Y \setminus X, X) = \sum_{P: \{Y \setminus X\}, X = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(t, X_i), \quad |X| \geq 0, \quad (57)$$

and hence we obtain expression (56) as a solution of recurrence relations (57).

In fact as above the following criterion is valid. Expansion (55) is a solution of the initial-value problem of the dual BBGKY hierarchy (53) if and only if the evolution operators  $\mathfrak{A}_{1+n}(t)$ ,  $n \geq 0$ , satisfy the recurrence relations (57).

We remark that an analog of expansion (19)-(20) in case of a solution of the dual BBGKY hierarchy (50) is given by expansion (55) with the following reduced cumulants of groups of operators (16)

$$U_{1+n}(t, \{x_1, \dots, x_{s-n}\}, x_{s-n+1}, \dots, x_s) = \sum_{k=0}^n (-1)^k \frac{n!}{k!(n-k)!} S_{s-k}(t). \quad (58)$$

In fact it is a consequence of the equivalence of corresponding generating functionals. Indeed, solving recurrence relations (57) with respect to the first-order cumulants for the separation terms which are independent from the variables  $Y \setminus X$

$$\mathfrak{A}_{1+n}(t, \{Y \setminus X\}, X) = \sum_{Z \subset X} \mathfrak{A}_1(t, \{Y \setminus X \cup Z\}) \sum_{P: X \setminus Z = \bigcup_i X_i} (-1)^{|P|} |P|! \prod_{i=1}^{|P|} \mathfrak{A}_1(t, \{X_i\}),$$

where  $\sum_{Z \subset X}$  is the sum over all possible subsets  $Z \subset X$  of the set  $X$ , and, taking into account the identity

$$\sum_{P: X \setminus Z = \bigcup_i X_i} (-1)^{|P|} |P|! \prod_{i=1}^{|P|} \mathfrak{A}_1(t, \{X_i\}) b_{s-n}(Y \setminus X) = \sum_{P: X \setminus Z = \bigcup_i X_i} (-1)^{|P|} |P|! b_{s-n}(Y \setminus X),$$

and the equality

$$\sum_{P: X \setminus Z = \bigcup_i X_i} (-1)^{|P|} |P|! = (-1)^{|X \setminus Z|},$$

we derive expansion (55) over reduced cumulants (58) of the dual BBGKY hierarchy (50).

We note that for certain classes of observables solution expansion (55) has more simple structure. As we can see from (48) one component sequences of marginal observables correspond to observables of certain structure, namely the marginal observable  $B^{(1)} = (0, a_1(x_1), 0, \dots)$  corresponds to the additive-type observable  $A^{(1)} = (0, a_1(x_1), \dots, \sum_{i=1}^n a_1(x_i), \dots)$ , and in the general case the  $k$ -ary-type marginal observable  $B^{(k)} = (0, \dots, 0, a_k(x_1, \dots, x_k), 0, \dots)$  corresponds to the  $k$ -ary-type observable  $A^{(k)} = (0, \dots, 0, a_k(x_1, \dots, x_k), \dots, \sum_{i_1 < \dots < i_k=1}^n a_s(x_{i_1}, \dots, x_{i_k}), \dots)$ . Then in case of additive-type observables solution expansion (55) attains the form

$$B_s^{(1)}(t, Y) = \mathfrak{A}_s(t, Y) \sum_{i=1}^s a_1(x_i),$$

where  $\mathfrak{A}_s(t, Y)$  is the  $sth$ -order cumulant (56) of groups of operators (16).

## 5 Conclusion

By means of established relations for generating functionals (7),(21),(34) and (46) the hierarchies of evolution equations in functional derivatives for generating functionals of marginal states and observables of classical many-particle systems, namely the BBGKY hierarchy for marginal distribution functions (10), the Liouville hierarchy (22) for correlation functions, the nonlinear BBGKY hierarchy for marginal correlation functions (37) and the dual BBGKY hierarchy for marginal observables (52), were derived from the Liouville equations in functional derivatives for generating functionals of distribution functions (5) and observables (51) respectively. To clarify the structure of these hierarchies in functional derivatives we generalized them for particles interacting via many body interaction potentials, in particular we have equations (13),(14) for states, equations (23),(38) for correlations of states and equations (51),(52) for observables.

On the basis of cluster expansions (17) and (54) of groups of operators which describe dynamics of finitely many particles the nonperturbative solutions of the hierarchies of evolution equations for states and observables were constructed. They are represented in the form of expansions (19) and (55) over particle clusters which evolution is governed by the corresponding order cumulant (18) of groups of operators (16) of the Liouville equations (6) in case of the BBGKY hierarchy (15) and cumulant (56) of groups of operators of the Liouville equations for observables (45) in case of the dual BBGKY hierarchy (53) respectively.

Moreover, along with the definition within the framework of the non-equilibrium grand canonical ensemble the marginal distribution functions can be defined in terms of dynamics of correlations (32) that allows, in particular to give the rigorous meaning of the states for more general classes of functions than the integrable functions. Using relation (34) of the generating functional of marginal correlation functions and the generating functional of correlation functions governed by the Liouville hierarchy (24), a nonperturbative solution of the nonlinear BBGKY hierarchy for marginal correlation functions (39) was constructed in the form of expansions (41) over particle clusters which evolution is governed by the corresponding order cumulant (42) of groups of operators (30) of the Liouville hierarchy (24).

Thus, the concept of cumulants of groups of operators forms the basis of established nonperturbative solution expansions of hierarchies of evolution equations of many-particle systems.

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